(7R,8S)-8-(4-Hydroxy-3-methoxyphenyl)-3-methox

Inchi: InChI=1S/C20H22O4/c1-11-7-14-9-19(24-4)17(22)10-15(14)20(12(11)2)13-5-6-16(21)18

InchiKey: XPWUEOIRZVEGJK-UHFFFAOYSA-N

Formula: C20H22O4

SMILES: COc1cc(C2c3cc(O)c(OC)cc3C=C(C)C2C)ccc1O

Mol. weight [g/mol]: 326.39

CAS: 135962-21-9

Physical Properties

Property code	Value	Unit	Source
gf	-144.52	kJ/mol	Joback Method
hf	-543.93	kJ/mol	Joback Method
hfus	46.35	kJ/mol	Joback Method
hvap	98.23	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.300		Crippen Method
mcvol	253.460	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	2659.80		NIST Webbook
rinpol	2659.80		NIST Webbook
tb	941.86	K	Joback Method
tc	1188.75	K	Joback Method
tf	696.92	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.06	J/mol×K	941.86	Joback Method
cpg	895.56	J/mol×K	1147.60	Joback Method
cpg	880.33	J/mol×K	1106.45	Joback Method
cpg	865.12	J/mol×K	1065.30	Joback Method
cpg	849.78	J/mol×K	1024.16	Joback Method
cpg	834.15	J/mol×K	983.01	Joback Method
cpg	910.97	J/mol×K	1188.75	Joback Method

dvisc	0.0000003	Pa×s	941.86	Joback Method
dvisc	0.0000004	Pa×s	901.04	Joback Method
dvisc	0.0000006	Pa×s	860.21	Joback Method
dvisc	0.0000009	Pa×s	819.39	Joback Method
dvisc	0.0000013	Pa×s	778.57	Joback Method
dvisc	0.0000021	Pa×s	737.74	Joback Method
dvisc	0.0000037	Pa×s	696.92	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C135962219&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume